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Mechanistic Modeling for Deriving Numeric Nutrient Criteria

Goal: Discuss the considerations needed to use and develop mechanistic models that integrate nutrient-sensitive assessment endpoints and water quality targets to derive numeric nutrient criteria

Outline

Mechanistic water quality models for nutrient criteria development:

- What are mechanistic models?
- Why should we use them?
- How do we use them?

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Mechanistic Water Quality Modeling

- EPA’s technical guidance:
  - Reference condition approach
  - Stressor-response analysis
  - Mechanistic modeling

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Mechanistic Water Quality Modeling

A Tool for Nutrient Criteria Development

- Reference condition approach
  - Ability to demonstrate minimally impacted waters
  - Sufficient nutrient data
- Stressor-response analysis
  - Paired stressor-response data
  - Sufficient data across all classes (each cofactor requires more data)
- Mechanistic modeling
  - Any water condition (doesn't require minimally impacted waters)
  - Ambient trend data (doesn't require paired data)
  - Models “borrow” information from neighboring segments

What is a Mechanistic Model?

- Collection of mathematical equations that represent chemical, physical, and biological mechanisms
  - Flow is a key mechanism for the delivery of contaminants and concentrations of contaminants
- Derived from the law of conservation:
  - Momentum
  - Heat energy
  - Water mass
  - Contaminant mass

Types of Mechanistic Models

1. Watershed Models

- Describe hydrologic mechanisms (e.g., flow)
- Describe delivery of contaminants from the watershed to a stream, river, lake, or estuary (e.g., temperature, total nitrogen, total phosphorus, total suspended solids, dissolved oxygen, biochemical oxygen demand)

2. Hydrodynamic Models

- Describe water movement (e.g., volume, velocity, direction); can describe the water movement in one, two, or three dimensions over varying time periods
- Simulate corresponding changes in properties (e.g., temperature and salinity)

3. Water Quality Models

- Describe changes that occur to contaminants (e.g., eutrophication models describe nutrient cycles; growth of algae; and production and consumption of dissolved oxygen)

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Why Model?

- Examine the interactions between nutrient loadings and response
- Test if assessment endpoints are sensitive to nutrients
- Predict nutrient condition for which water quality data are either insufficient or unavailable
- Explore candidate nutrient criteria
- Provide a methodology that can be duplicated and is credible and defensible

Why Model?

Models provide spatial information to help understand the water system and the changes in nutrient concentrations from upstream to downstream.

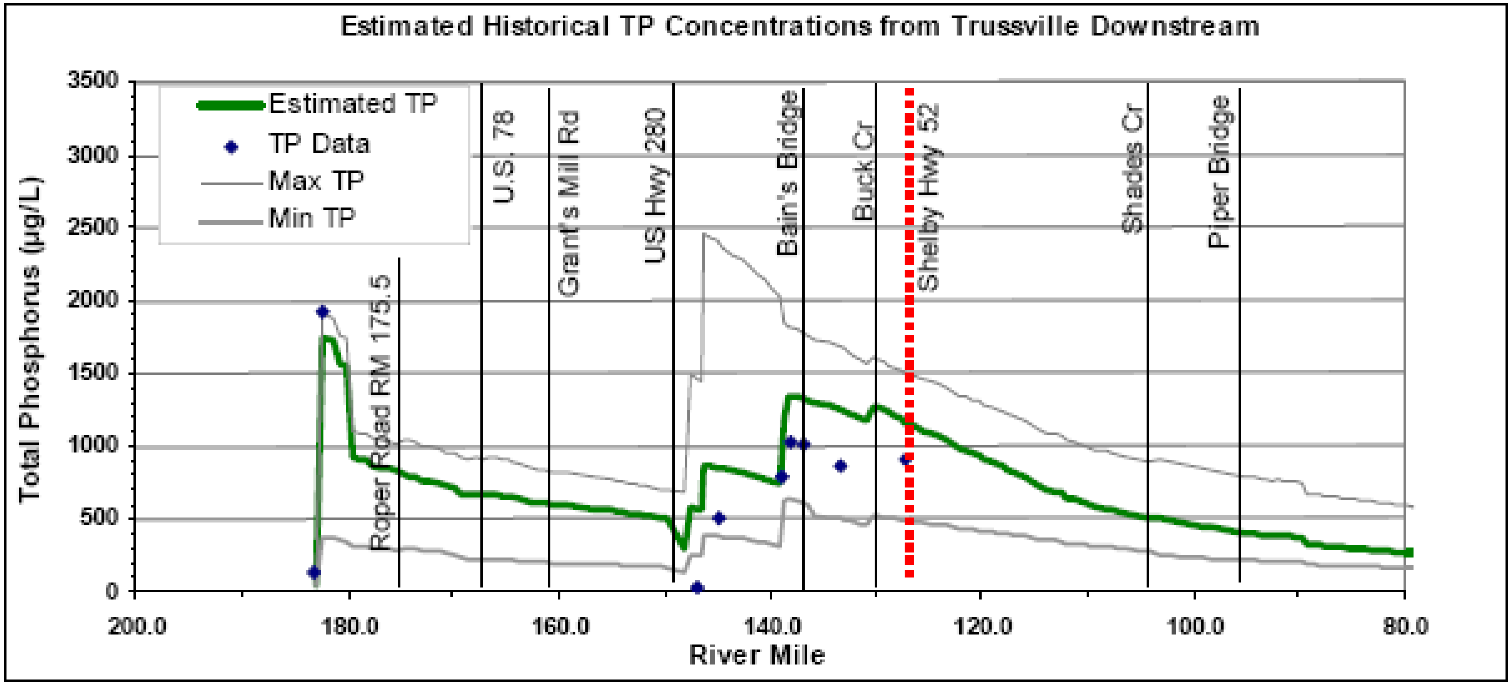
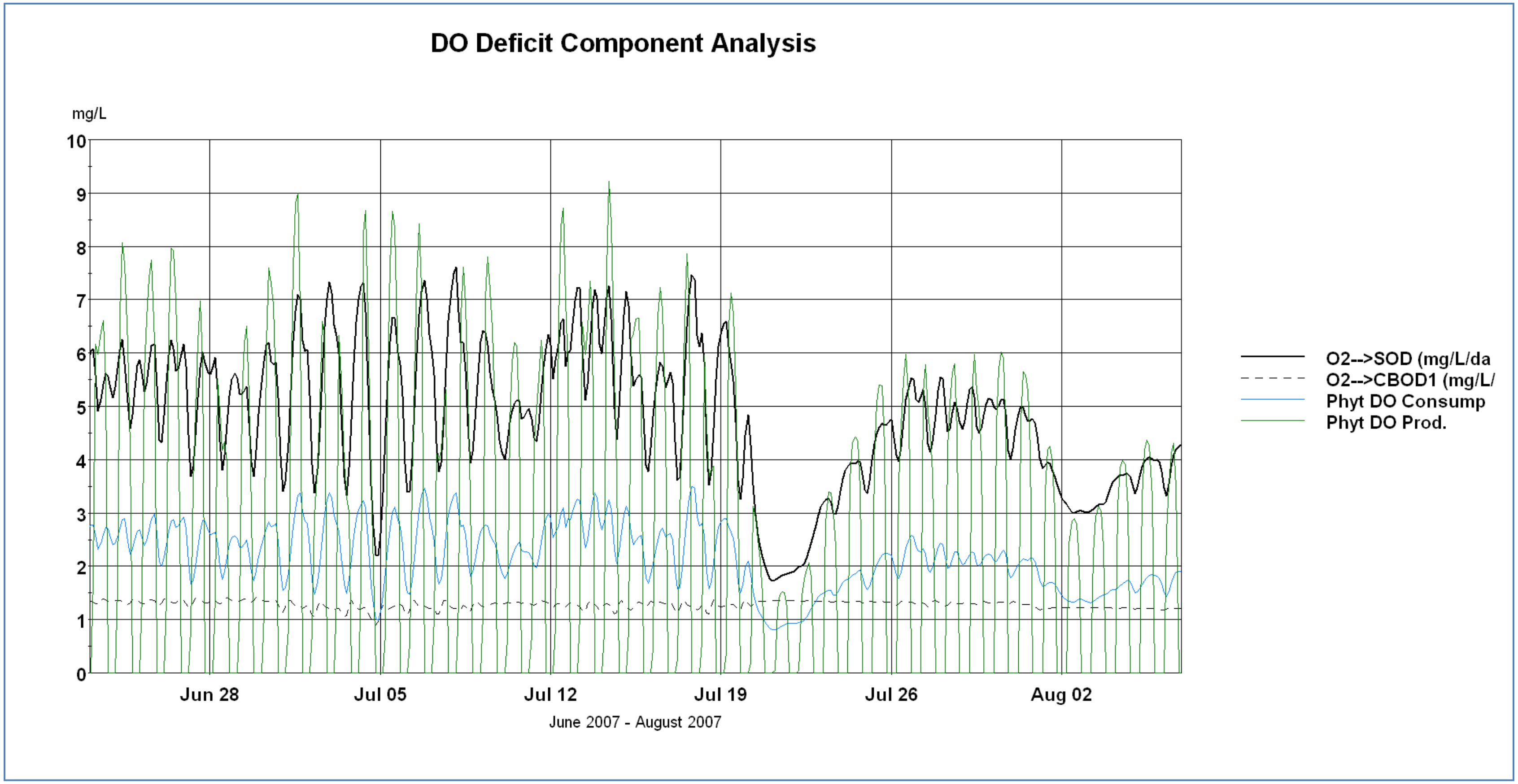


Figure 4-12 Estimated Monthly-Median Total Phosphorus Concentrations in the Cahaba River in September 1999, from Trussville to Centreville

Why Model?

Models provide component analysis and insight into which processes impact the assessment endpoint(s).



How to Use Water Quality Models

1. **Define** targets
2. **Select** a model that includes processes important to the water quality target
3. **Collect** additional data to inform the model
4. **Configure**
5. **Calibrate**
6. **Run** scenarios
7. **Apply** model results to interpret assessment endpoint targets and calculate nutrient criteria values

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Step 1. Define Targets

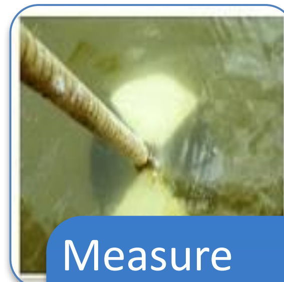
Example: SAV Target

Management Goal

- Maintain SAV communities

Assessment Endpoint

- SAV depth of colonization



Measure

- Depth
- Light

Target (model state variable)

- Light attenuation coefficient

Step 1. Define Targets

Chlorophyll-a:

- Daily average concentration at the surface < 20µg/L
  90 percent of the time

Dissolved oxygen:

- Daily water column average
- Instantaneous (model output interval) water column average
- Bottom instantaneous to check against hypoxia

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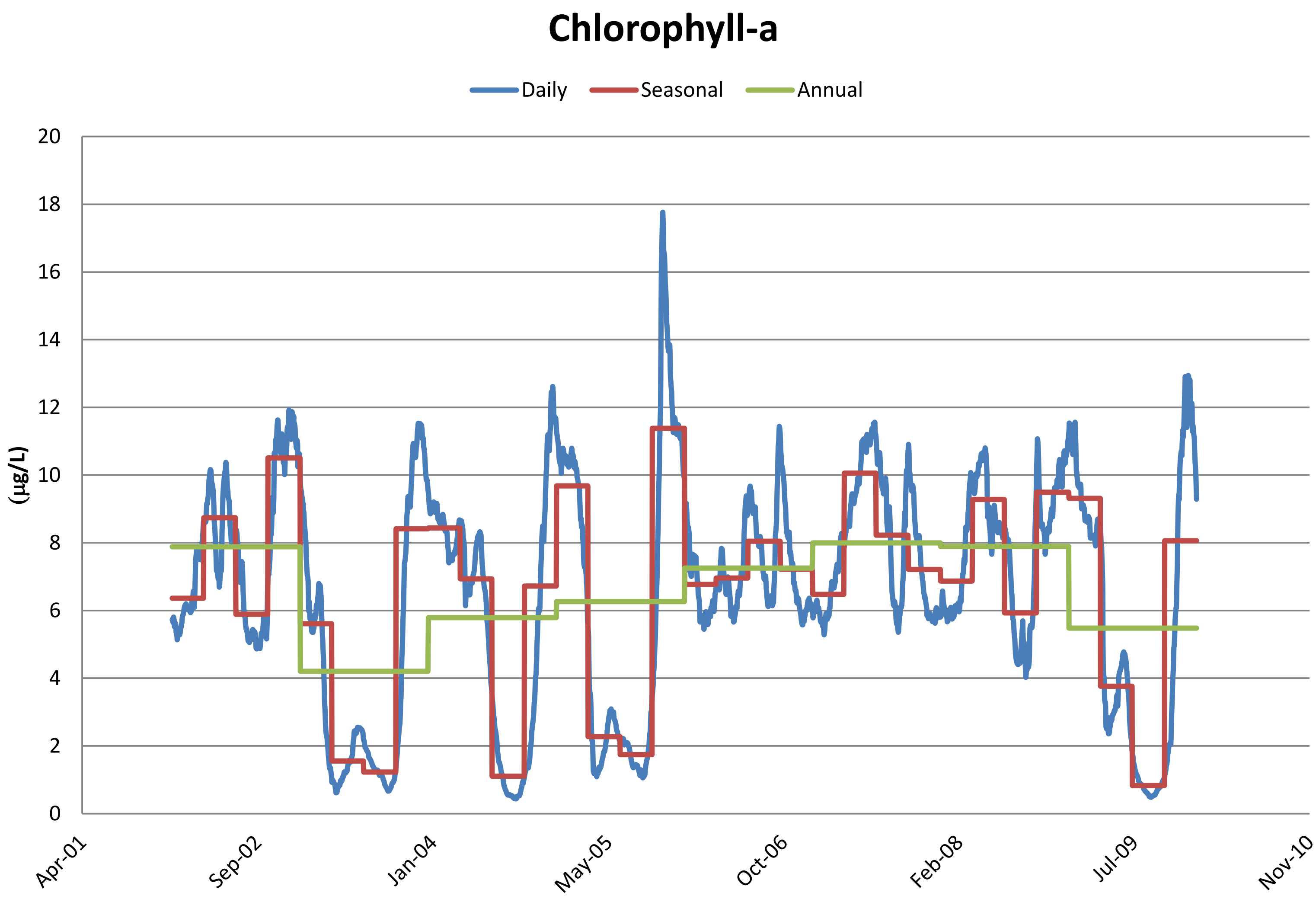
Step 2. Select Model

- Model selection should be a collaborative decision among model experts, stakeholders, and other experts.
- Model should be as simple as possible.
- Model should be complex enough to:
  - Address spatial and temporal considerations
  - Include important mechanisms

Step 2. Select Model

Temporal Considerations



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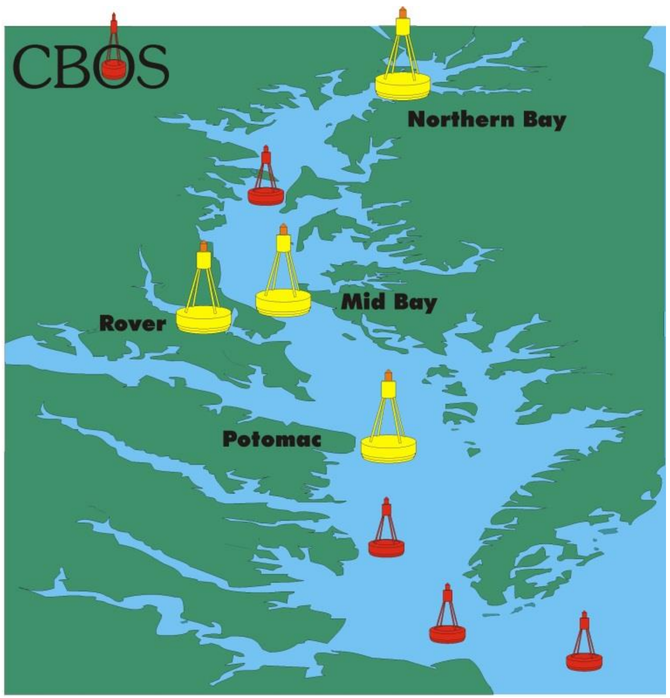
Step 3. Collect Data

- Data are needed to inform each process
- Flow and water surface elevation
- Salinity

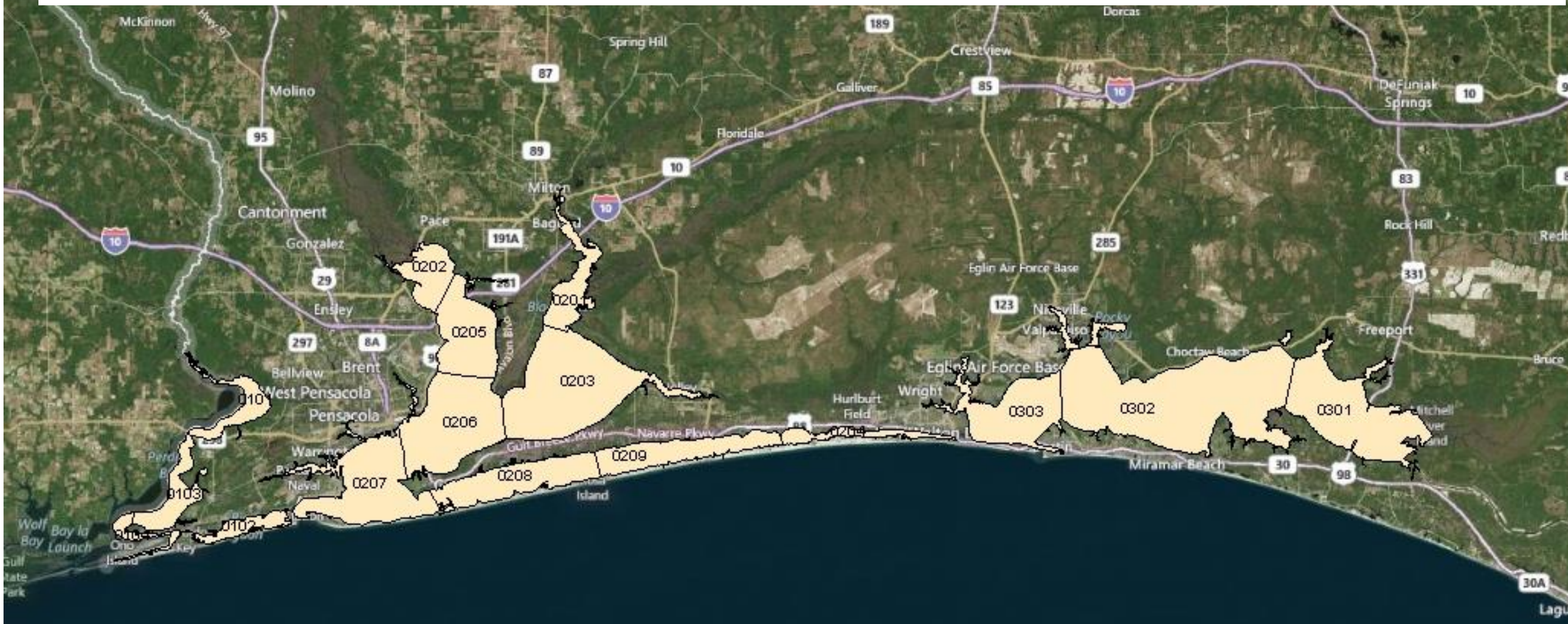


- Dissolved Oxygen:
  - Biochemical oxygen demand or organic carbon
  - Nitrogen: ammonia, nitrate, organic
  - Reaeration
  - Sediment oxygen demand
  - Algal production and respiration and phosphorus

- Water Clarity:
  - Colored dissolved organic matter
  - Algae
  - Suspended solids
  - Light attenuation measurements

Configure the Model

Segmenting Large Waterbodies

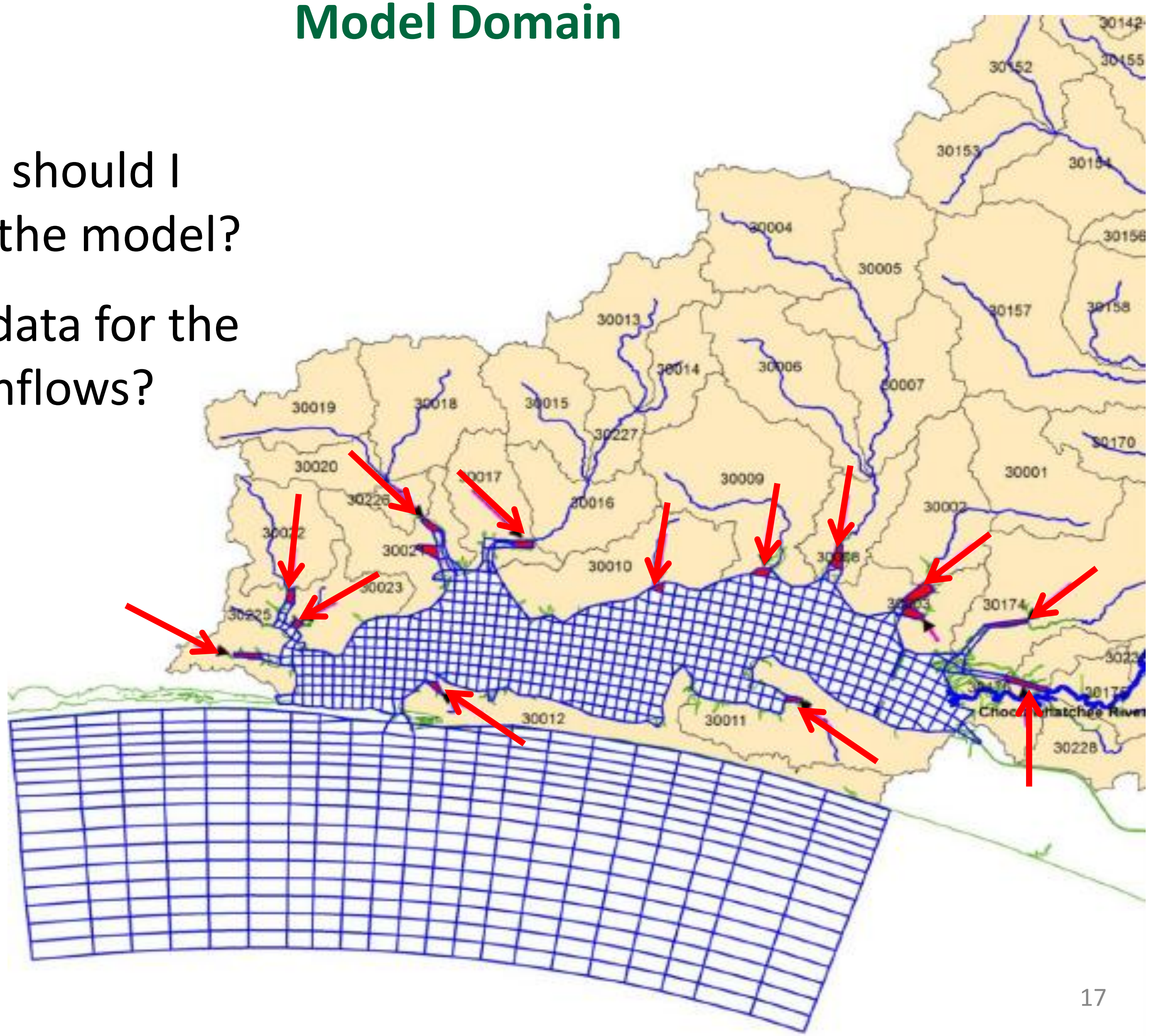


Salinity, physical features such as bridges and causeways, SAV coverage, and depth distribution considered when segmenting each estuary to account for hydrology and ecosystem dynamics.

Step 4. Configure the Model

Model Domain

- What area should I include in the model?
- Do I have data for the tributary inflows?

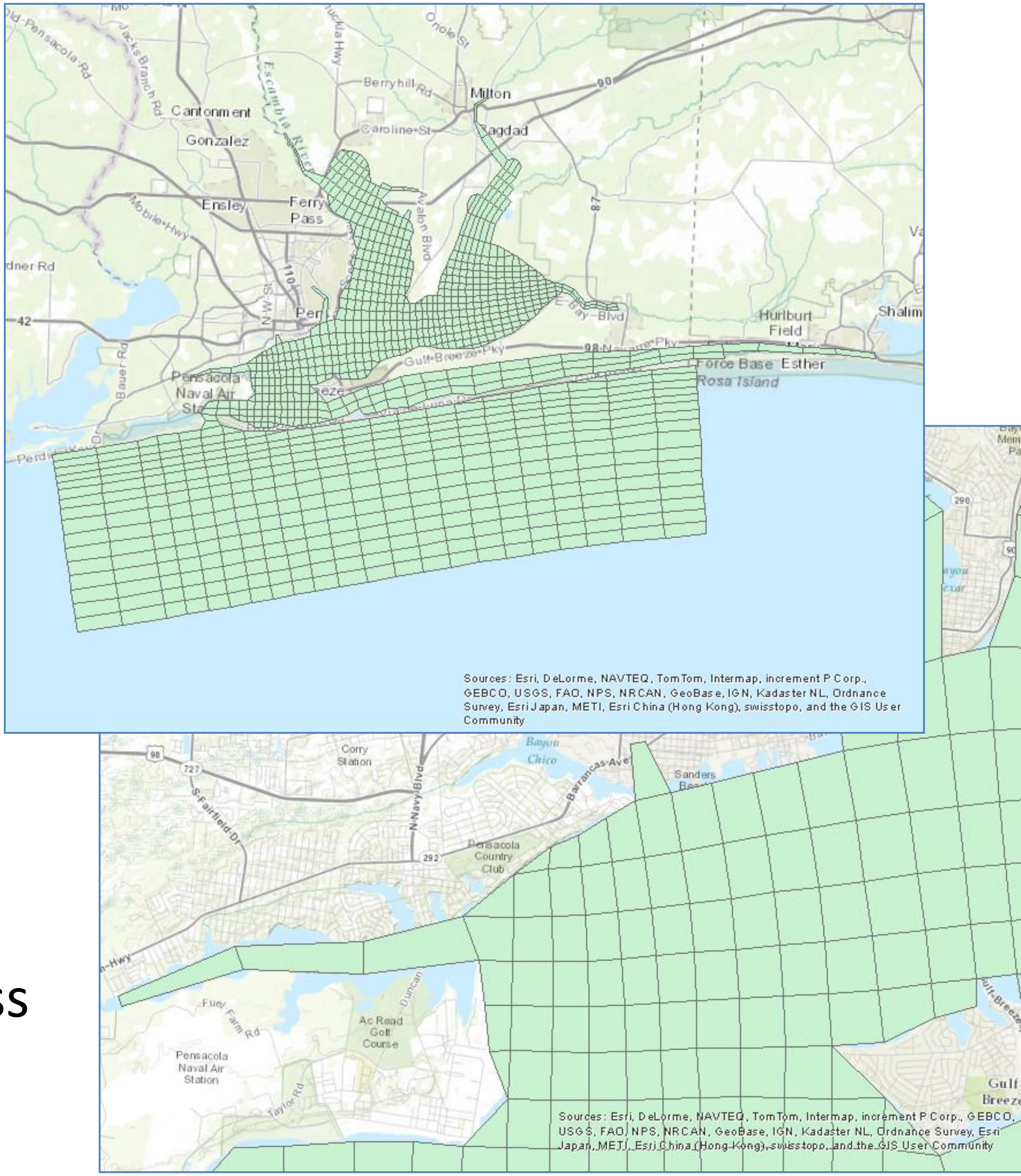


Step 4. Configure the Model
Model Domain

Should I model the entire watershed?

Step 4. Configure the Model

- Physical parameters (geometry and forcing functions)
  - Grid resolution:
    - Main estuary
    - Small embayments
    - Tidal creeks
- Boundary conditions
- Loadings
- Kinetic rates, constants for each biological process



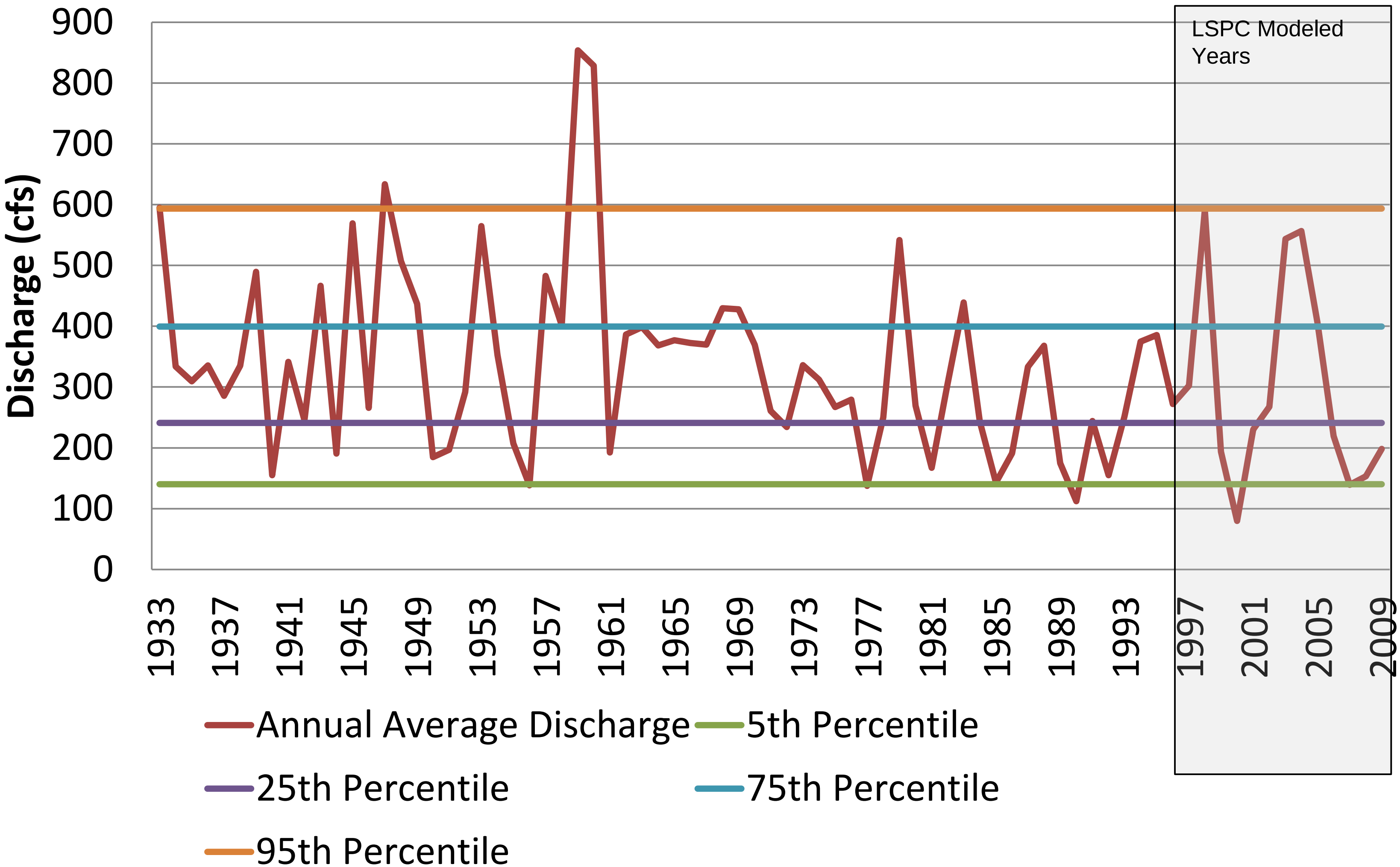
Step 4. Configure the Model

Kinetic Rates and Constants

- Nitrification Rate Constant at 20 °C
- Half Saturation Constant for Nitrification Oxygen Limit (mg/L)
- Denitrification Rate Constant at 20 °C
- Dissolved Organic Nitrogen Mineralization Rate Constant
- Mineralization Rate Constant for Dissolved Organic Phosphorus
- Fraction of Phytoplankton Death Recycled to Organic Phosphorus
- Phytoplankton Maximum Quantum Yield Constant
- Phytoplankton Optimal Light Saturation
- Background Light Extinction Multiplier
- Detritus and Solids Light Extinction Multiplier
- Dissolved Organic Carbon Light Extinction Multiplier

Step 4. Configure the Model

Time Period Based on Expected Hydrology

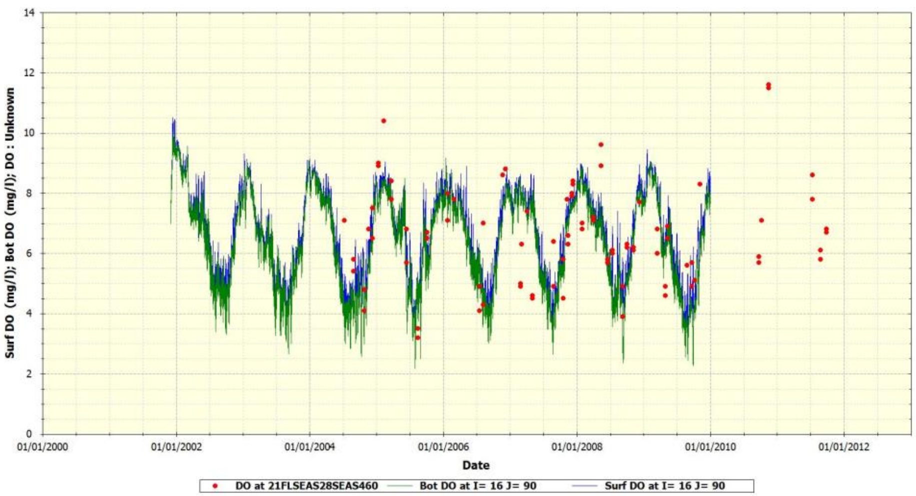


Step 5. Calibration

- Calibration is adjusting kinetic parameters until predictions match observed data
- Four approaches to assessing model error:
  - Visual comparison of model results and observations with plots
  - Statistical tests
  - Sensitivity analysis
  - Error analysis (Monte Carlo analysis)

Step 5. Calibration

Calibration Plots and Error Statistics



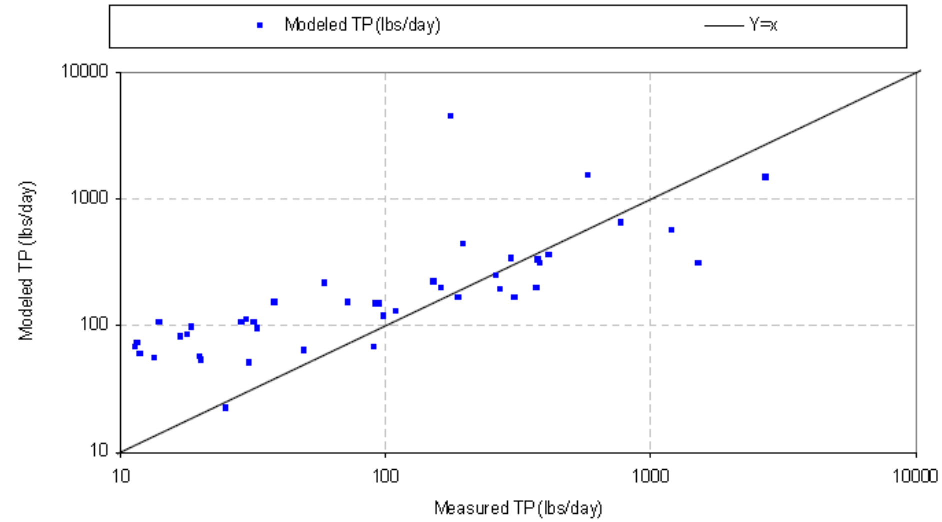


Figure C2-48. TP (lbs/day) load scatter plot at 21FLBFA 33040004

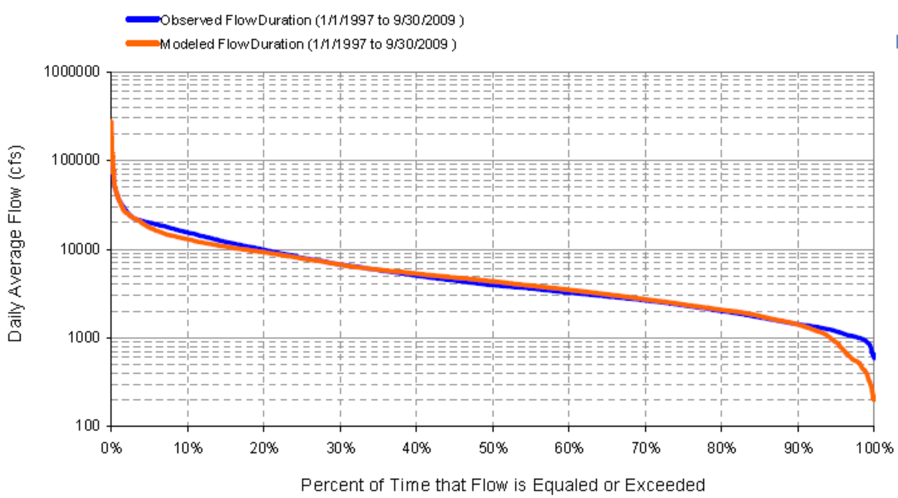


Figure C2-21. Flow exceedance: Model Outlet 20028 vs. USGS 02376033 Escambia River near Molino, FL (USGS No date)

$$Average\ Error = \frac{1}{N}\sum_{i=1}^{N}(O_i - S_i)$$

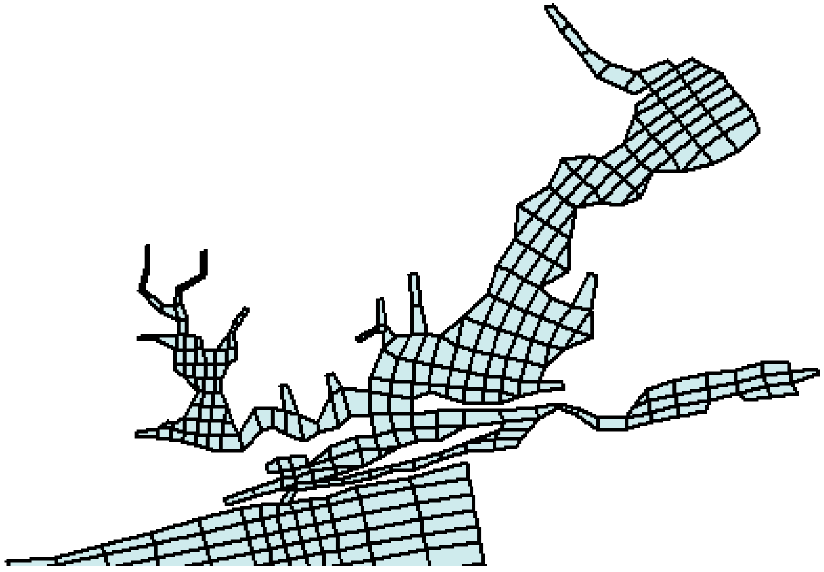
$$RMS\ Error = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(O_i - S_i)^2}$$

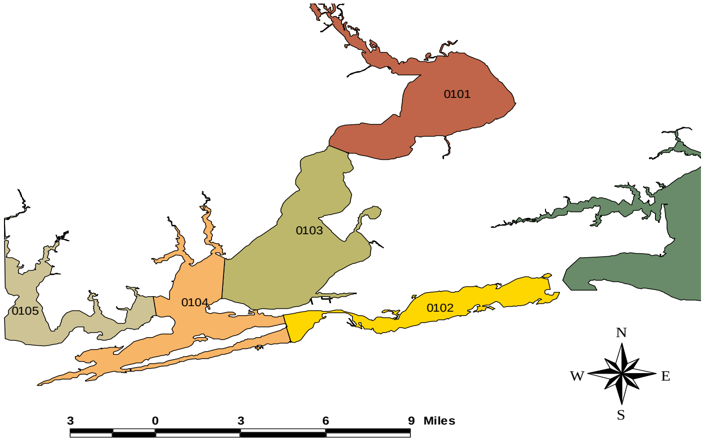
Step 6. Run Scenarios

- Configure and run “Use Support” scenarios
- Evaluate levels of nutrient loading and the estuary response
- Explore unmeasured inputs, rates, boundary conditions, constants, and processes

Step 7. Apply Model Results

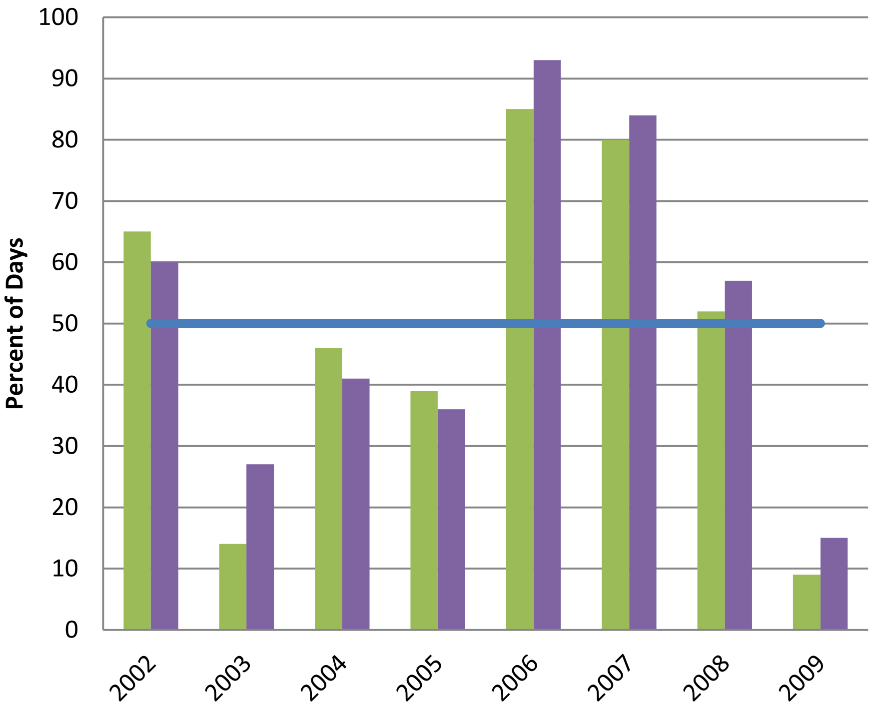
- Evaluate model results
  - Interpret assessment endpoint targets
  - Calculate nutrient criteria values
- Perform post-processing of output and compute metrics (segment averaged chlorophyll-a and dissolved oxygen concentrations, light attenuation)



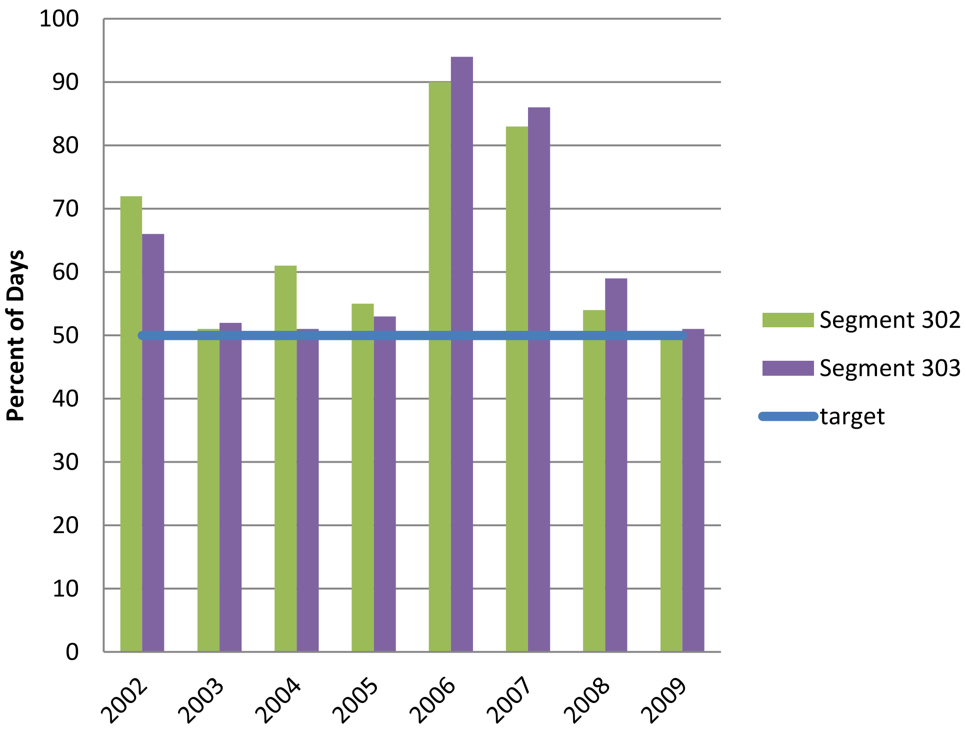


Step 7. Apply Model Results

Percent of Days with 20% Light under Current Load Conditions

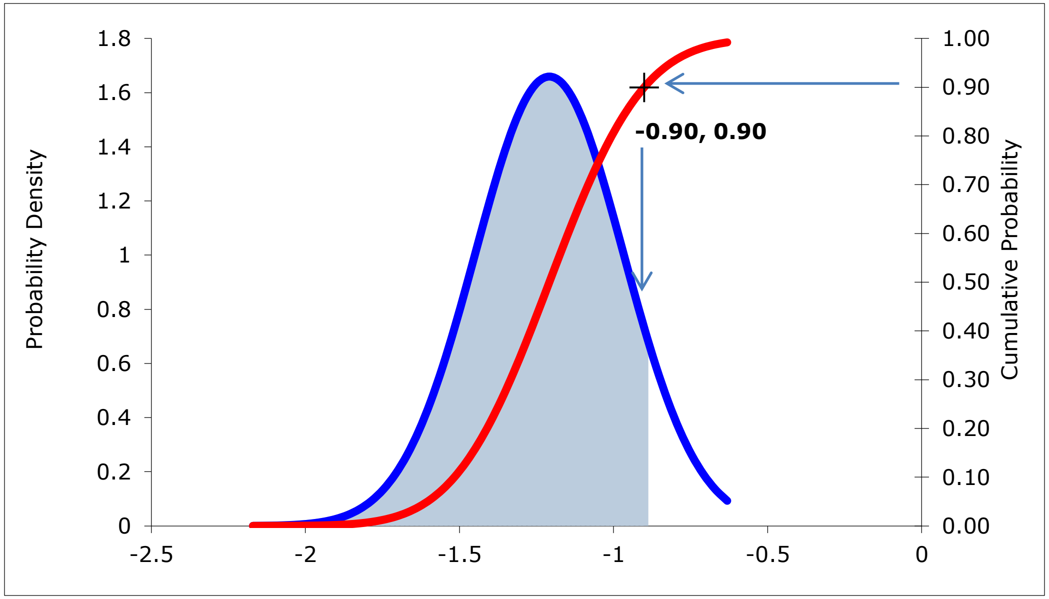


Percent of Days with 20% Light under Reduced Load Conditions



Step 7. Apply Model Results

Calculate upper end of distribution of annual average of natural logarithms:



Calculate values exceeded only once out of three years:

Year	Total Nitrogen (mg/L) - Annual Geomeans	Value Exceeded Once in Three Years
2002	0.29	
2003	0.42	
2004	0.33	0.33
2005	0.31	0.33
2006	0.21	0.31
2007	0.22	0.22
2008	0.29	0.22
2009	0.38	0.29
		0.33

Lessons Learned

Mechanistic models:

- Describe water movement, better understand water quality dynamics, and link nutrients with their sources
- Test if assessment endpoints are sensitive to nutrients
- Explore candidate nutrient criteria
- Evaluate downstream effects
- Provide a methodology that can be duplicated and is credible and defensible